



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:39 AM EDT

PDB ID : 2GMJ / pdb_00002gmj
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.
Deposited on : 2006-04-06
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

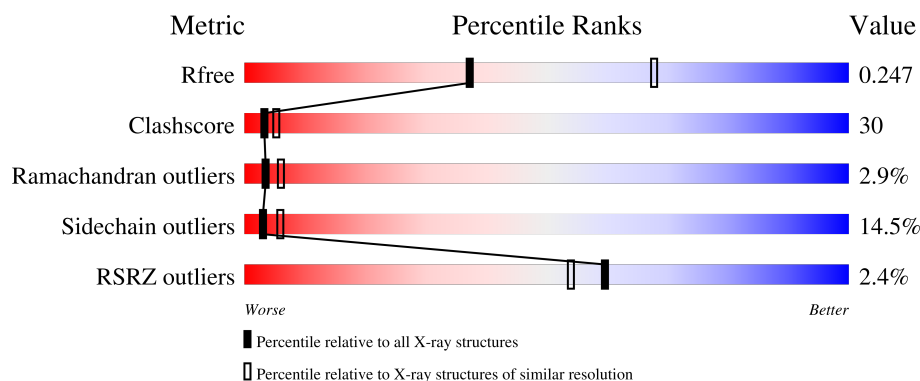
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	584	4% 59% 29% 10% ..
1	B	584	4% 40% 45% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	B	612	-	-	X	-

2 Entry composition [i](#)

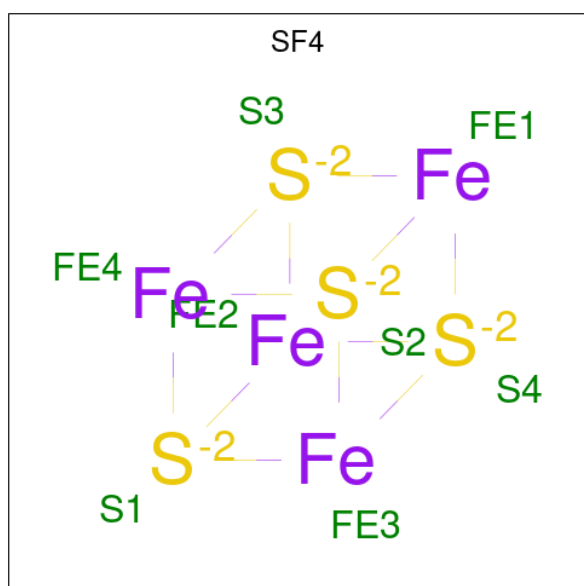
There are 5 unique types of molecules in this entry. The entry contains 9345 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Electron transfer flavoprotein-ubiquinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4553	2907	791	835	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



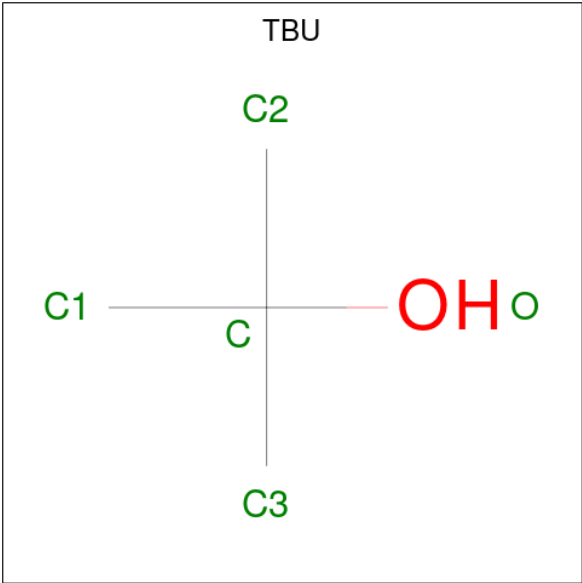
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is TERTIARY-BUTYL ALCOHOL (CCD ID: TBU) (formula: C₄H₁₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	4	1		
4	A	1	Total	C	O	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	4	1		
4	A	1	Total	C	O	0	0
			5	4	1		
4	B	1	Total	C	O	0	0
			5	4	1		
4	B	1	Total	C	O	0	0
			5	4	1		

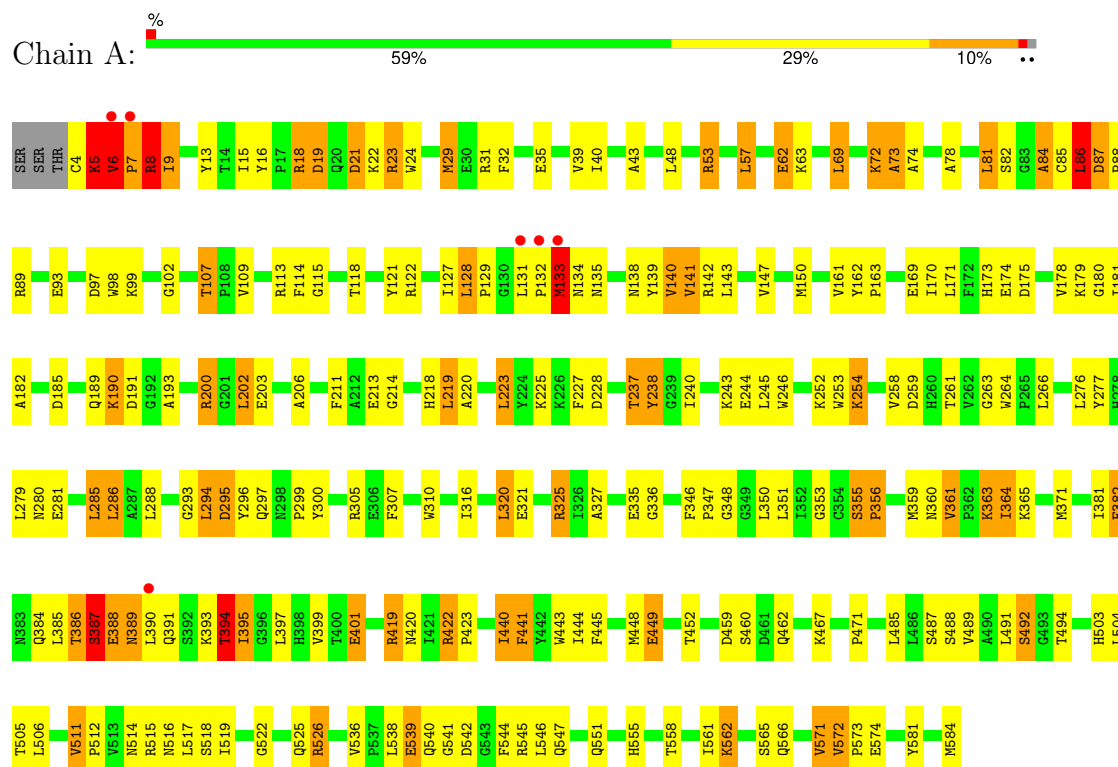
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	32	Total	O	0	0
			32	32		

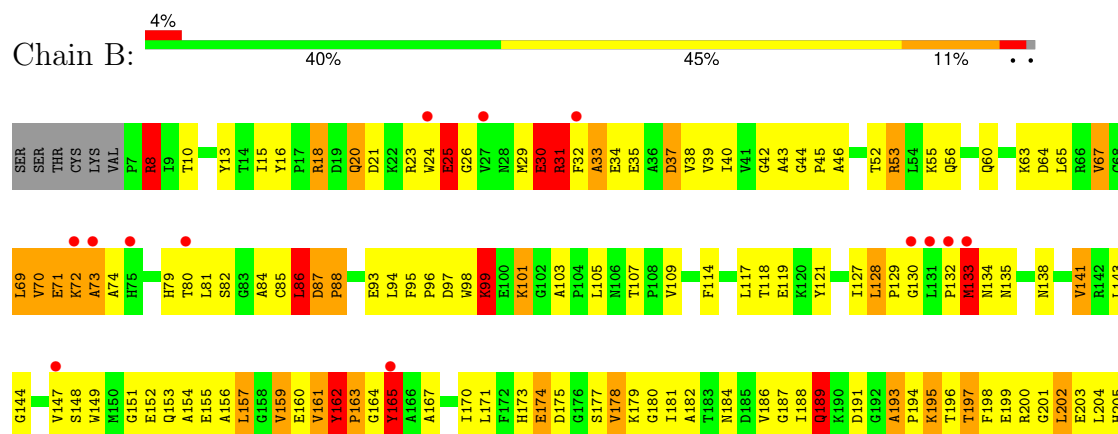
3 Residue-property plots

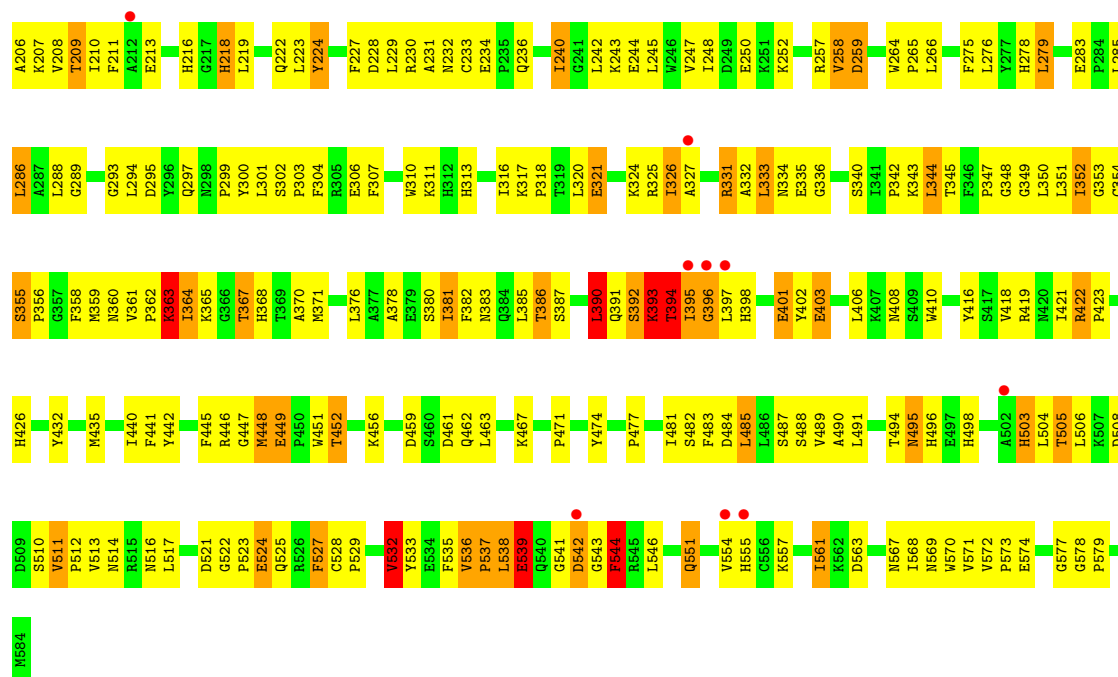
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase



• Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.84Å 154.84Å 130.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.60 28.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	78.9 (28.75-2.60) 78.8 (28.75-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.255 0.221 , 0.247	Depositor DCC
R_{free} test set	3135 reflections (7.73%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9345	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FAD, TBU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.59	1/4682 (0.0%)	1.19	47/6356 (0.7%)
1	B	0.54	1/4660 (0.0%)	1.26	51/6326 (0.8%)
All	All	0.57	2/9342 (0.0%)	1.22	98/12682 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	MET	SD-CE	6.95	1.97	1.79
1	B	193	ALA	CA-CB	5.71	1.61	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	GLY	N-CA-C	-13.95	91.78	110.20
1	B	536	VAL	N-CA-C	11.30	120.03	108.95
1	B	73	ALA	N-CA-C	11.26	123.58	108.38
1	B	196	THR	N-CA-C	-10.86	99.22	111.82
1	B	193	ALA	CA-C-N	10.79	133.32	119.84
1	B	193	ALA	C-N-CA	10.79	133.32	119.84
1	B	162	TYR	CA-C-N	10.38	132.81	119.84
1	B	162	TYR	C-N-CA	10.38	132.81	119.84
1	B	536	VAL	CA-C-N	10.09	132.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	VAL	C-N-CA	10.09	132.45	119.84
1	B	544	PHE	N-CA-C	9.78	131.62	110.80
1	B	396	GLY	N-CA-C	-9.40	96.88	111.64
1	B	393	LYS	N-CA-C	-9.10	91.42	110.80
1	A	98	TRP	N-CA-C	8.69	120.75	111.28
1	A	5	LYS	N-CA-C	8.21	128.28	110.80
1	A	16	TYR	CA-C-N	7.83	128.31	119.93
1	A	16	TYR	C-N-CA	7.83	128.31	119.93
1	B	87	ASP	CA-C-N	7.75	129.53	119.84
1	B	87	ASP	C-N-CA	7.75	129.53	119.84
1	B	128	LEU	CA-C-N	7.58	129.32	119.84
1	B	128	LEU	C-N-CA	7.58	129.32	119.84
1	A	394	THR	N-CA-C	-7.46	94.91	110.80
1	A	6	VAL	N-CA-C	7.43	124.92	108.88
1	A	87	ASP	CA-C-N	7.24	126.95	119.56
1	A	87	ASP	C-N-CA	7.24	126.95	119.56
1	A	85	CYS	N-CA-C	-7.23	95.37	108.02
1	B	390	LEU	N-CA-C	7.21	120.96	110.28
1	B	63	LYS	N-CA-C	-7.08	100.99	110.55
1	B	224	TYR	CA-C-N	7.04	129.71	120.28
1	B	224	TYR	C-N-CA	7.04	129.71	120.28
1	B	93	GLU	N-CA-C	-6.92	103.84	112.90
1	A	487	SER	N-CA-C	-6.91	103.80	111.82
1	A	562	LYS	N-CA-C	6.86	121.40	112.89
1	B	321	GLU	N-CA-C	-6.82	99.81	109.96
1	B	165	TYR	N-CA-C	6.76	121.28	107.69
1	B	86	LEU	N-CA-C	6.75	120.08	109.96
1	A	102	GLY	N-CA-C	6.73	123.67	114.92
1	B	8	ARG	N-CA-C	6.73	125.14	110.80
1	A	441	PHE	N-CA-C	6.72	120.93	112.87
1	B	381	ILE	N-CA-C	-6.65	104.03	110.42
1	A	355	SER	N-CA-C	-6.59	103.51	112.35
1	A	390	LEU	N-CA-C	6.59	119.85	109.96
1	B	189	GLN	N-CA-C	6.54	120.28	110.14
1	A	32	PHE	N-CA-C	-6.53	101.74	110.55
1	B	326	ILE	N-CA-C	6.43	118.28	112.17
1	A	8	ARG	N-CA-C	-6.41	97.14	110.80
1	A	162	TYR	CA-C-N	-6.33	113.76	120.03
1	A	162	TYR	C-N-CA	-6.33	113.76	120.03
1	B	352	ILE	CB-CA-C	-6.33	105.79	111.74
1	B	31	ARG	N-CA-C	6.25	119.21	109.52
1	A	238	TYR	N-CA-C	6.25	118.06	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	LEU	CA-C-N	6.20	125.90	119.82
1	A	128	LEU	C-N-CA	6.20	125.90	119.82
1	A	385	LEU	N-CA-C	-6.18	105.89	113.50
1	A	361	VAL	N-CA-C	6.03	119.59	112.35
1	A	572	VAL	CA-C-N	6.03	127.36	120.85
1	A	572	VAL	C-N-CA	6.03	127.36	120.85
1	A	391	GLN	N-CA-C	-6.00	97.36	107.99
1	B	532	VAL	N-CA-C	5.95	121.71	109.34
1	A	516	ASN	N-CA-C	5.94	117.44	110.97
1	B	387	SER	N-CA-C	-5.91	106.20	113.41
1	A	118	THR	N-CA-C	-5.90	100.44	109.41
1	B	56	GLN	N-CA-C	-5.84	104.91	111.28
1	B	367	THR	N-CA-C	5.83	117.31	111.07
1	B	155	GLU	N-CA-C	-5.81	106.04	113.01
1	B	394	THR	N-CA-C	-5.80	98.44	110.80
1	B	247	VAL	N-CA-C	-5.79	99.30	107.75
1	A	19	ASP	N-CA-C	-5.78	105.99	113.16
1	B	355	SER	N-CA-C	-5.75	104.64	112.35
1	A	121	TYR	N-CA-C	5.68	118.51	109.81
1	A	74	ALA	N-CA-C	-5.68	104.45	111.33
1	A	73	ALA	N-CA-C	5.65	118.21	110.24
1	B	32	PHE	N-CA-C	-5.61	103.13	110.53
1	A	492	SER	N-CA-C	-5.60	106.80	113.97
1	A	86	LEU	N-CA-C	5.53	118.83	109.76
1	B	163	PRO	N-CA-C	5.50	123.80	112.47
1	B	25	GLU	N-CA-C	5.48	120.42	111.37
1	B	232	ASN	N-CA-C	5.48	117.01	110.44
1	B	107	THR	CA-C-N	-5.47	114.34	120.14
1	B	107	THR	C-N-CA	-5.47	114.34	120.14
1	A	519	ILE	N-CA-C	5.39	116.05	110.82
1	A	297	GLN	N-CA-C	5.35	119.89	112.45
1	B	363	LYS	N-CA-C	-5.33	106.77	113.28
1	A	140	VAL	N-CA-C	-5.31	100.77	108.36
1	A	84	ALA	N-CA-C	5.29	122.07	110.80
1	A	141	VAL	N-CA-C	5.28	114.97	108.53
1	B	121	TYR	N-CA-C	5.27	117.28	109.69
1	B	386	THR	N-CA-C	5.27	119.68	112.88
1	A	395	ILE	N-CA-C	-5.24	106.19	113.00
1	B	401	GLU	N-CA-C	-5.22	106.06	112.90
1	B	561	ILE	N-CA-C	5.19	115.86	110.82
1	A	460	SER	N-CA-C	5.13	116.88	111.28
1	A	285	LEU	N-CA-C	5.13	118.17	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ALA	N-CA-C	5.12	116.94	108.13
1	A	382	PHE	N-CA-C	-5.11	105.71	111.28
1	A	93	GLU	N-CA-C	-5.05	105.68	111.14
1	A	295	ASP	N-CA-C	-5.05	106.96	112.72
1	B	539	GLU	N-CA-C	5.03	121.50	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4553	0	4450	179	0
1	B	4531	0	4424	377	0
2	A	8	0	0	0	0
2	B	8	0	0	3	0
3	A	53	0	30	2	0
3	B	53	0	30	3	0
4	A	20	0	40	5	0
4	B	10	0	20	0	0
5	A	77	0	0	2	0
5	B	32	0	0	1	0
All	All	9345	0	8994	556	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PRO:HB3	1:B:546:LEU:HD13	1.18	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:CE1	1:B:219:LEU:HG	1.88	1.08
1:B:393:LYS:HA	1:B:393:LYS:CE	1.83	1.06
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.38	1.05
1:B:299:PRO:HG3	1:B:463:LEU:HD22	1.41	1.02
1:B:524:GLU:HA	1:B:527:PHE:CE1	2.01	0.96
1:B:503:HIS:HB2	1:B:571:VAL:O	1.66	0.96
1:B:55:LYS:HG3	1:B:159:VAL:HG12	1.46	0.95
1:B:325:ARG:NH2	1:B:488:SER:HA	1.82	0.94
1:A:441:PHE:HB3	1:A:449:GLU:OE2	1.66	0.93
1:B:39:VAL:HG23	1:B:206:ALA:HB2	1.49	0.92
1:B:99:LYS:H	1:B:99:LYS:HD2	1.33	0.91
1:B:512:PRO:CB	1:B:546:LEU:HD13	1.99	0.91
1:B:55:LYS:HB3	1:B:157:LEU:HD12	1.54	0.90
1:A:364:ILE:HD11	4:A:621:TBU:H13	1.50	0.90
1:B:535:PHE:CZ	1:B:546:LEU:HD12	2.06	0.89
1:A:21:ASP:OD2	1:A:23:ARG:HD3	1.74	0.88
1:A:445:PHE:O	1:A:448:MET:HG3	1.73	0.87
1:B:419:ARG:NH1	1:B:452:THR:HG22	1.89	0.86
1:B:390:LEU:H	1:B:390:LEU:HD22	1.39	0.86
1:B:175:ASP:OD2	1:B:394:THR:HA	1.77	0.85
1:B:189:GLN:HG3	1:B:193:ALA:O	1.76	0.85
1:A:133:MET:HA	1:A:133:MET:CE	2.05	0.85
1:B:361:VAL:HG11	1:B:422:ARG:HG3	1.55	0.85
1:B:394:THR:O	1:B:396:GLY:N	2.08	0.85
1:B:8:ARG:HG3	1:B:8:ARG:HH11	1.39	0.85
1:B:195:LYS:HG2	1:B:197:THR:OG1	1.77	0.85
1:B:224:TYR:HA	1:B:229:LEU:HD12	1.57	0.85
1:B:178:VAL:HG22	1:B:348:GLY:HA3	1.59	0.84
1:A:522:GLY:O	1:A:525:GLN:HG2	1.77	0.83
1:B:286:LEU:HD23	1:B:288:LEU:HD21	1.60	0.82
1:B:31:ARG:HD2	1:B:201:GLY:O	1.79	0.81
1:B:325:ARG:HH22	1:B:488:SER:HA	1.43	0.81
1:B:363:LYS:O	1:B:365:LYS:HD3	1.80	0.81
1:A:39:VAL:HG23	1:A:206:ALA:HB2	1.63	0.81
1:A:492:SER:OG	1:A:494:THR:HG22	1.81	0.81
1:B:43:ALA:HB3	1:B:71:GLU:HG2	1.63	0.81
1:A:7:PRO:HD2	1:A:9:ILE:CG1	2.11	0.80
1:B:512:PRO:HB3	1:B:546:LEU:CD1	2.08	0.80
1:A:393:LYS:O	1:A:394:THR:HG23	1.81	0.80
1:B:218:HIS:HE1	1:B:219:LEU:HG	1.46	0.80
1:B:419:ARG:HH11	1:B:452:THR:HG22	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:VAL:HG23	1:B:208:VAL:O	1.82	0.79
1:A:7:PRO:HD2	1:A:9:ILE:HG12	1.64	0.78
1:B:393:LYS:HA	1:B:393:LYS:HE2	1.62	0.78
1:A:131:LEU:HD13	4:A:623:TBU:H32	1.64	0.77
1:B:202:LEU:HD13	1:B:203:GLU:N	2.00	0.77
1:B:84:ALA:HB3	1:B:141:VAL:O	1.85	0.77
1:B:496:HIS:CD2	1:B:578:GLY:H	2.02	0.77
1:A:351:LEU:HB3	1:A:356:PRO:HG3	1.66	0.77
1:B:510:SER:O	1:B:514:ASN:HB2	1.83	0.76
1:A:364:ILE:CD1	4:A:621:TBU:H13	2.16	0.75
1:B:40:ILE:HB	1:B:69:LEU:HD23	1.68	0.75
1:A:355:SER:HB3	1:A:356:PRO:HD3	1.68	0.75
1:B:114:PHE:HB2	1:B:127:ILE:HD11	1.67	0.75
1:B:440:ILE:HG22	1:B:441:PHE:N	1.99	0.75
1:B:441:PHE:HB3	1:B:449:GLU:OE2	1.89	0.73
1:B:496:HIS:HD2	1:B:577:GLY:HA3	1.54	0.73
1:B:508:ASP:HB3	1:B:511:VAL:CG1	2.18	0.73
1:B:504:LEU:HD21	2:B:612:SF4:S4	2.28	0.73
1:A:107:THR:HG23	1:A:280:ASN:HB3	1.70	0.73
1:B:445:PHE:O	1:B:448:MET:HG2	1.89	0.72
1:B:535:PHE:CE2	1:B:546:LEU:HD12	2.24	0.72
1:A:361:VAL:HG11	1:A:422:ARG:HG3	1.71	0.72
1:A:173:HIS:CE1	1:A:179:LYS:HG3	2.25	0.71
1:A:353:GLY:O	1:A:356:PRO:HD2	1.90	0.71
1:A:87:ASP:HA	1:A:138:ASN:OD1	1.90	0.71
1:B:55:LYS:CB	1:B:157:LEU:HD12	2.20	0.71
1:A:386:THR:HG22	1:A:386:THR:O	1.90	0.71
1:B:345:THR:HB	1:B:398:HIS:NE2	2.05	0.71
1:B:82:SER:CB	1:B:143:LEU:HD12	2.21	0.71
1:A:170:ILE:HD13	1:A:223:LEU:HD13	1.71	0.71
1:A:218:HIS:CE1	1:A:219:LEU:HD13	2.26	0.70
1:B:171:LEU:HD11	1:B:203:GLU:HG3	1.72	0.70
1:B:334:ASN:HD21	1:B:354:CYS:HB3	1.54	0.70
1:B:310:TRP:CZ2	1:B:316:ILE:HD13	2.26	0.70
1:A:294:LEU:HD11	1:A:558:THR:HG23	1.74	0.70
1:A:5:LYS:HD3	1:A:6:VAL:HG12	1.73	0.70
1:A:539:GLU:H	1:A:539:GLU:CD	2.00	0.70
1:A:388:GLU:O	1:A:389:ASN:C	2.33	0.70
1:B:390:LEU:HD22	1:B:390:LEU:N	2.06	0.70
1:B:344:LEU:HB2	1:B:402:TYR:HE1	1.56	0.69
1:A:175:ASP:OD2	1:A:395:ILE:HG13	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:LYS:HB3	1:B:368:HIS:HE1	1.56	0.69
1:A:132:PRO:O	1:A:363:LYS:HG3	1.91	0.69
1:B:209:THR:HG23	1:B:211:PHE:HE1	1.57	0.69
1:B:351:LEU:O	1:B:352:ILE:HG23	1.92	0.69
1:B:276:LEU:HG	1:B:288:LEU:HD22	1.75	0.69
1:B:275:PHE:CE2	1:B:289:GLY:HA3	2.28	0.68
1:B:160:GLU:HB3	1:B:162:TYR:HE1	1.58	0.68
1:B:161:VAL:CG2	1:B:163:PRO:HD3	2.23	0.68
1:B:160:GLU:HB3	1:B:162:TYR:CE1	2.28	0.68
1:B:33:ALA:HB2	1:B:203:GLU:HB3	1.74	0.68
1:B:95:PHE:CE2	1:B:149:TRP:HZ3	2.12	0.68
1:B:394:THR:C	1:B:396:GLY:H	2.02	0.67
1:B:392:SER:O	1:B:393:LYS:HB2	1.92	0.67
1:A:401:GLU:CD	1:A:401:GLU:H	2.01	0.67
1:A:440:ILE:HG22	1:A:441:PHE:N	2.09	0.67
1:B:208:VAL:CG2	1:B:397:LEU:HB2	2.25	0.67
1:B:355:SER:HB3	1:B:356:PRO:HD3	1.77	0.67
1:B:161:VAL:HG23	1:B:163:PRO:HD3	1.77	0.67
1:B:132:PRO:O	1:B:363:LYS:HD2	1.94	0.66
1:B:364:ILE:HG12	1:B:364:ILE:O	1.96	0.66
1:B:43:ALA:CB	1:B:71:GLU:HG2	2.25	0.66
1:B:8:ARG:HG3	1:B:8:ARG:NH1	2.11	0.66
1:A:29:MET:O	1:A:200:ARG:HD2	1.96	0.65
1:A:387:SER:O	1:A:388:GLU:HB2	1.96	0.65
1:B:325:ARG:HH22	1:B:488:SER:CA	2.08	0.65
1:A:133:MET:HA	1:A:133:MET:HE2	1.78	0.65
1:A:15:ILE:HD12	1:A:505:THR:HB	1.77	0.65
1:B:297:GLN:O	1:B:463:LEU:HD23	1.96	0.65
1:B:202:LEU:HD12	1:B:204:LEU:HG	1.79	0.65
1:B:335:GLU:HA	1:B:361:VAL:HG22	1.78	0.65
1:B:365:LYS:HB3	1:B:368:HIS:CE1	2.31	0.65
1:B:334:ASN:ND2	1:B:354:CYS:HB3	2.12	0.65
1:A:150:MET:HE1	1:A:371:MET:HE2	1.79	0.65
1:B:242:LEU:N	1:B:242:LEU:HD12	2.12	0.64
1:B:441:PHE:CD2	1:B:449:GLU:HG2	2.33	0.64
1:B:177:SER:OG	1:B:394:THR:O	2.13	0.64
1:A:294:LEU:O	1:A:459:ASP:HB3	1.98	0.64
1:B:154:ALA:HB1	1:B:159:VAL:HG21	1.79	0.64
1:B:213:GLU:OE1	1:B:219:LEU:HB2	1.98	0.64
1:A:485:LEU:O	1:A:489:VAL:HG23	1.96	0.64
1:B:317:LYS:HB3	1:B:318:PRO:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:CB	1:B:356:PRO:HG3	2.21	0.64
1:A:360:ASN:CG	1:A:363:LYS:HD3	2.22	0.64
1:B:248:ILE:HG21	1:B:286:LEU:HD22	1.78	0.64
1:B:170:ILE:CG1	1:B:219:LEU:HD22	2.28	0.64
1:B:203:GLU:HG2	1:B:205:HIS:HE1	1.61	0.64
1:B:99:LYS:H	1:B:99:LYS:CD	2.07	0.63
1:A:128:LEU:HB3	1:A:129:PRO:HD2	1.79	0.63
1:A:133:MET:HA	1:A:133:MET:HE3	1.79	0.63
1:B:208:VAL:HG13	1:B:349:GLY:HA2	1.79	0.63
1:B:393:LYS:CE	1:B:393:LYS:CA	2.68	0.63
1:A:243:LYS:NZ	1:A:584:MET:OXT	2.32	0.63
1:A:7:PRO:HD2	1:A:9:ILE:HG13	1.80	0.63
1:A:360:ASN:ND2	1:A:363:LYS:HD3	2.14	0.62
1:B:202:LEU:HD13	1:B:203:GLU:H	1.62	0.62
1:B:257:ARG:HD3	1:B:259:ASP:OD1	1.99	0.62
1:B:242:LEU:HD22	1:B:304:PHE:HA	1.81	0.62
1:A:73:ALA:HB1	1:A:78:ALA:HB3	1.80	0.62
1:B:300:TYR:CD2	1:B:471:PRO:HA	2.35	0.62
1:A:325:ARG:HD3	1:A:491:LEU:HD12	1.81	0.62
1:B:363:LYS:O	1:B:364:ILE:HG22	2.01	0.61
1:B:72:LYS:NZ	1:B:79:HIS:ND1	2.49	0.61
1:B:72:LYS:HB2	3:B:613:FAD:C4A	2.29	0.60
1:B:82:SER:HB3	1:B:143:LEU:HD12	1.82	0.60
1:B:494:THR:HA	1:B:578:GLY:O	2.02	0.60
1:B:189:GLN:CG	1:B:193:ALA:O	2.48	0.60
1:B:245:LEU:HD23	1:B:286:LEU:O	2.01	0.60
1:B:179:LYS:HE2	1:B:205:HIS:CD2	2.37	0.60
1:A:40:ILE:HB	1:A:69:LEU:HD22	1.84	0.60
1:A:335:GLU:HA	1:A:361:VAL:HG21	1.82	0.60
1:A:350:LEU:HD21	1:A:399:VAL:HB	1.84	0.60
1:B:495:ASN:C	1:B:495:ASN:HD22	2.09	0.60
1:B:72:LYS:HE2	1:B:555:HIS:CD2	2.36	0.59
1:B:344:LEU:CD1	1:B:403:GLU:HG2	2.32	0.59
1:A:335:GLU:HA	1:A:361:VAL:CG2	2.33	0.59
1:B:98:TRP:NE1	1:B:99:LYS:HE2	2.17	0.59
1:B:208:VAL:HG23	1:B:397:LEU:HB2	1.84	0.59
1:A:24:TRP:CE3	1:A:29:MET:HE1	2.37	0.59
1:B:40:ILE:O	1:B:70:VAL:HG23	2.02	0.59
1:B:285:LEU:H	1:B:285:LEU:HD23	1.68	0.59
1:B:243:LYS:HG2	1:B:244:GLU:N	2.16	0.59
1:B:317:LYS:HE3	1:B:481:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:HIS:CE1	1:B:179:LYS:HG3	2.37	0.59
1:B:523:PRO:HB2	1:B:527:PHE:CE2	2.38	0.59
1:B:24:TRP:HH2	1:B:198:PHE:CE1	2.21	0.59
1:B:498:HIS:CE1	1:B:551:GLN:HE21	2.21	0.59
1:B:186:VAL:HG12	1:B:187:GLY:N	2.18	0.58
1:B:344:LEU:HD21	1:B:358:PHE:HZ	1.67	0.58
1:B:505:THR:HG23	1:B:569:ASN:O	2.03	0.58
1:B:209:THR:CG2	1:B:211:PHE:HE1	2.15	0.58
1:B:294:LEU:O	1:B:459:ASP:HB3	2.03	0.58
1:B:536:VAL:O	1:B:544:PHE:HA	2.02	0.58
1:A:350:LEU:HD11	1:A:381:ILE:HD11	1.85	0.58
1:B:31:ARG:HG2	1:B:200:ARG:HB3	1.85	0.58
1:B:300:TYR:CE2	1:B:471:PRO:HG3	2.39	0.58
1:A:7:PRO:CD	1:A:9:ILE:HG12	2.31	0.58
1:B:37:ASP:OD1	1:B:207:LYS:HE3	2.03	0.58
1:B:344:LEU:CD2	1:B:358:PHE:HZ	2.17	0.58
1:B:174:GLU:OE1	1:B:174:GLU:HA	2.04	0.58
1:B:310:TRP:CE2	1:B:316:ILE:HD13	2.38	0.58
1:B:324:LYS:NZ	1:B:326:ILE:HG22	2.20	0.57
1:B:325:ARG:HH12	1:B:483:PHE:HB2	1.70	0.57
1:B:86:LEU:HD22	1:B:87:ASP:N	2.18	0.57
1:B:276:LEU:HG	1:B:288:LEU:CD2	2.34	0.57
1:B:432:TYR:HA	1:B:435:MET:HE3	1.86	0.57
1:A:189:GLN:HG2	1:A:193:ALA:O	2.04	0.57
1:B:230:ARG:HA	1:B:233:CYS:SG	2.45	0.57
1:A:511:VAL:N	1:A:512:PRO:HD2	2.20	0.57
1:B:21:ASP:HB3	1:B:24:TRP:HD1	1.69	0.57
1:A:43:ALA:HB2	1:A:69:LEU:HD11	1.87	0.57
1:A:202:LEU:HD13	1:A:203:GLU:H	1.70	0.57
1:B:72:LYS:NZ	1:B:72:LYS:HB3	2.20	0.57
1:B:333:LEU:N	1:B:333:LEU:HD23	2.19	0.57
1:B:363:LYS:O	1:B:364:ILE:CG2	2.53	0.57
1:B:178:VAL:HG22	1:B:348:GLY:CA	2.34	0.56
1:B:351:LEU:HB3	1:B:356:PRO:CG	2.26	0.56
1:A:517:LEU:HA	1:A:522:GLY:N	2.21	0.56
1:B:13:TYR:HB2	1:B:18:ARG:HD2	1.87	0.56
1:B:55:LYS:HE2	1:B:67:VAL:CG1	2.36	0.56
1:B:195:LYS:HB3	1:B:198:PHE:H	1.71	0.56
1:B:512:PRO:O	1:B:516:ASN:HB2	2.06	0.56
1:B:175:ASP:OD2	1:B:394:THR:CA	2.51	0.56
1:B:496:HIS:HA	5:B:783:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HA	1:B:522:GLY:N	2.20	0.56
1:B:132:PRO:HG2	1:B:133:MET:SD	2.46	0.56
1:A:350:LEU:CD1	1:A:381:ILE:HD11	2.36	0.56
1:B:10:THR:O	1:B:16:TYR:HE1	1.88	0.56
1:B:511:VAL:HG13	1:B:512:PRO:HD3	1.87	0.56
1:A:142:ARG:HD3	1:A:281:GLU:OE1	2.06	0.56
1:B:244:GLU:OE2	1:B:311:LYS:NZ	2.28	0.55
1:B:495:ASN:O	1:B:495:ASN:ND2	2.38	0.55
1:A:300:TYR:CE2	1:A:471:PRO:HG3	2.41	0.55
1:A:517:LEU:HA	1:A:522:GLY:H	1.70	0.55
1:B:180:GLY:O	1:B:181:ILE:HD12	2.05	0.55
1:B:243:LYS:CG	1:B:244:GLU:N	2.69	0.55
1:B:517:LEU:HD22	1:B:535:PHE:CD2	2.41	0.55
1:B:70:VAL:HG12	1:B:165:TYR:O	2.07	0.55
1:B:24:TRP:HH2	1:B:198:PHE:HE1	1.55	0.54
1:B:508:ASP:HB3	1:B:511:VAL:HG12	1.87	0.54
1:B:203:GLU:HG2	1:B:205:HIS:CE1	2.42	0.54
1:B:257:ARG:HG2	1:B:258:VAL:N	2.22	0.54
1:B:511:VAL:O	1:B:512:PRO:C	2.51	0.54
1:B:35:GLU:O	1:B:35:GLU:HG2	2.07	0.54
1:B:85:CYS:O	1:B:365:LYS:HE3	2.08	0.54
1:B:426:HIS:CE1	1:B:456:LYS:HG3	2.43	0.54
1:B:485:LEU:O	1:B:489:VAL:HG23	2.07	0.54
1:B:25:GLU:HG3	1:B:26:GLY:N	2.23	0.54
1:B:151:GLY:O	1:B:154:ALA:HB3	2.08	0.54
1:B:275:PHE:CZ	1:B:289:GLY:HA3	2.42	0.54
1:A:13:TYR:HB3	1:A:18:ARG:HD3	1.90	0.54
1:B:42:GLY:O	1:B:43:ALA:HB3	2.06	0.54
1:B:182:ALA:HA	1:B:202:LEU:O	2.08	0.54
1:A:107:THR:HG23	1:A:280:ASN:CB	2.38	0.54
1:B:353:GLY:O	1:B:356:PRO:HD2	2.08	0.53
1:B:503:HIS:H	1:B:503:HIS:CD2	2.24	0.53
1:B:324:LYS:HZ2	1:B:326:ILE:HG22	1.73	0.53
1:A:211:PHE:HB2	1:A:351:LEU:HD23	1.90	0.53
1:B:394:THR:C	1:B:396:GLY:N	2.63	0.53
1:A:53:ARG:NH2	1:A:57:LEU:HD13	2.24	0.53
1:B:344:LEU:HD13	1:B:403:GLU:HG2	1.88	0.53
1:A:539:GLU:O	1:A:540:GLN:HB2	2.08	0.53
1:B:18:ARG:HG3	1:B:29:MET:HE1	1.89	0.53
1:B:393:LYS:HA	1:B:393:LYS:HE3	1.85	0.53
1:B:451:TRP:CD1	1:B:451:TRP:C	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:C	1:B:101:LYS:H	2.15	0.53
1:B:170:ILE:HG13	1:B:219:LEU:HD22	1.91	0.53
1:B:208:VAL:HA	1:B:348:GLY:O	2.09	0.53
1:A:84:ALA:HB2	5:A:792:HOH:O	2.08	0.53
1:B:381:ILE:O	1:B:385:LEU:HG	2.09	0.53
1:A:364:ILE:HD11	4:A:621:TBU:C1	2.30	0.52
1:A:310:TRP:CE2	1:A:316:ILE:HD13	2.44	0.52
1:A:131:LEU:HD21	1:A:443:TRP:HB2	1.92	0.52
1:B:24:TRP:CH2	1:B:198:PHE:CE1	2.98	0.52
1:B:344:LEU:HD12	1:B:344:LEU:H	1.74	0.52
1:A:7:PRO:O	1:A:8:ARG:CB	2.58	0.52
1:B:34:GLU:H	1:B:202:LEU:HD11	1.74	0.52
1:B:46:ALA:HB2	1:B:370:ALA:HB1	1.91	0.52
1:B:188:ILE:HG22	1:B:189:GLN:N	2.24	0.52
1:B:419:ARG:HH11	1:B:452:THR:CG2	2.21	0.51
1:A:15:ILE:HD13	1:A:506:LEU:O	2.10	0.51
1:B:85:CYS:SG	1:B:135:ASN:OD1	2.68	0.51
1:B:325:ARG:NH1	1:B:483:PHE:HB2	2.25	0.51
1:B:288:LEU:HD11	1:B:320:LEU:HD23	1.90	0.51
1:B:363:LYS:C	1:B:364:ILE:HG22	2.36	0.51
1:B:80:THR:HG21	1:B:147:VAL:HG21	1.92	0.51
1:B:368:HIS:HD2	1:B:410:TRP:CH2	2.28	0.51
1:B:390:LEU:H	1:B:390:LEU:CD2	2.18	0.51
1:A:18:ARG:HH22	1:A:200:ARG:HH21	1.58	0.51
1:A:131:LEU:HD13	4:A:623:TBU:C3	2.36	0.51
1:A:293:GLY:C	1:A:295:ASP:H	2.18	0.51
1:B:301:LEU:HD23	1:B:302:SER:N	2.25	0.51
1:B:511:VAL:HG22	1:B:512:PRO:N	2.25	0.51
1:B:406:LEU:C	1:B:408:ASN:H	2.18	0.51
1:B:40:ILE:HB	1:B:69:LEU:CD2	2.39	0.51
1:B:175:ASP:OD1	1:B:175:ASP:N	2.44	0.51
1:B:55:LYS:NZ	1:B:65:LEU:O	2.39	0.51
1:B:351:LEU:O	1:B:352:ILE:CG2	2.59	0.51
1:B:483:PHE:N	1:B:483:PHE:CD1	2.79	0.50
1:B:508:ASP:O	1:B:511:VAL:HG13	2.11	0.50
1:A:401:GLU:N	1:A:401:GLU:OE2	2.42	0.50
1:A:29:MET:C	1:A:200:ARG:HD2	2.36	0.50
1:A:72:LYS:HG3	3:A:611:FAD:C4A	2.41	0.50
1:A:143:LEU:O	1:A:147:VAL:HG23	2.12	0.50
1:A:384:GLN:HE22	1:A:399:VAL:HA	1.76	0.50
1:B:79:HIS:CD2	1:B:579:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:CA	1:B:138:ASN:HD22	2.24	0.50
1:B:143:LEU:O	1:B:144:GLY:C	2.55	0.50
1:B:482:SER:C	1:B:483:PHE:HD1	2.20	0.50
1:B:179:LYS:HE2	1:B:205:HIS:NE2	2.27	0.50
1:A:258:VAL:HG13	1:A:277:TYR:CE2	2.46	0.49
1:A:348:GLY:N	1:A:397:LEU:O	2.35	0.49
1:A:299:PRO:O	1:A:526:ARG:HD2	2.11	0.49
1:B:82:SER:HB2	1:B:143:LEU:HD12	1.94	0.49
1:B:177:SER:HB3	1:B:394:THR:HB	1.94	0.49
1:B:325:ARG:NH1	1:B:483:PHE:CD2	2.81	0.49
1:B:393:LYS:CA	1:B:393:LYS:HE3	2.42	0.49
1:B:340:SER:O	1:B:342:PRO:HD3	2.13	0.49
1:B:521:ASP:OD1	1:B:521:ASP:O	2.31	0.49
1:B:154:ALA:HB1	1:B:159:VAL:CG2	2.40	0.49
1:A:31:ARG:HE	1:A:200:ARG:NH1	2.11	0.49
1:A:276:LEU:HD21	1:A:286:LEU:HD21	1.94	0.49
1:B:86:LEU:O	1:B:88:PRO:HD3	2.11	0.49
1:B:230:ARG:NH1	1:B:234:GLU:O	2.46	0.49
1:A:325:ARG:NH2	1:A:488:SER:OG	2.41	0.49
1:B:33:ALA:CB	1:B:203:GLU:HB3	2.41	0.49
1:B:38:VAL:CG1	1:B:67:VAL:HB	2.43	0.49
1:A:246:TRP:O	1:A:285:LEU:HD12	2.12	0.49
1:B:180:GLY:C	1:B:181:ILE:HD12	2.38	0.49
1:B:97:ASP:O	1:B:101:LYS:HB2	2.12	0.49
1:B:135:ASN:C	1:B:138:ASN:HD22	2.21	0.49
1:B:447:GLY:HA2	1:B:449:GLU:OE2	2.13	0.49
1:B:477:PRO:HB3	1:B:483:PHE:O	2.13	0.49
1:A:214:GLY:O	1:A:355:SER:HA	2.13	0.48
1:A:246:TRP:CE2	1:A:325:ARG:HB2	2.48	0.48
1:A:18:ARG:NH2	1:A:200:ARG:HH21	2.10	0.48
1:A:213:GLU:OE2	1:A:219:LEU:HB2	2.14	0.48
1:A:237:THR:HG23	1:A:336:GLY:HA2	1.96	0.48
1:A:263:GLY:O	1:A:264:TRP:C	2.55	0.48
1:B:157:LEU:HD13	1:B:157:LEU:O	2.13	0.48
1:B:135:ASN:HA	1:B:138:ASN:HD22	1.78	0.48
1:A:31:ARG:HH22	1:A:169:GLU:CD	2.21	0.48
1:B:161:VAL:HG22	1:B:163:PRO:HD3	1.95	0.48
1:B:484:ASP:OD2	1:B:487:SER:HB3	2.13	0.48
1:A:360:ASN:ND2	1:A:363:LYS:CD	2.76	0.48
1:B:248:ILE:HD13	1:B:286:LEU:HD13	1.94	0.48
1:B:382:PHE:CD1	1:B:382:PHE:C	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CD2	1:B:149:TRP:HZ3	2.31	0.48
1:B:118:THR:O	1:B:119:GLU:C	2.56	0.47
1:B:484:ASP:OD2	1:B:484:ASP:C	2.57	0.47
1:A:422:ARG:N	1:A:423:PRO:CD	2.77	0.47
1:B:149:TRP:CH2	1:B:153:GLN:HG3	2.49	0.47
1:B:181:ILE:CG2	1:B:182:ALA:N	2.76	0.47
1:A:440:ILE:O	1:A:444:ILE:HB	2.15	0.47
1:B:98:TRP:HB2	1:B:103:ALA:CB	2.44	0.47
1:A:62:GLU:C	1:A:63:LYS:HG2	2.40	0.47
1:A:109:VAL:HG23	1:A:138:ASN:O	2.15	0.47
1:A:113:ARG:HB2	1:A:259:ASP:OD1	2.15	0.47
1:A:355:SER:N	1:A:356:PRO:CD	2.77	0.47
1:A:538:LEU:O	1:A:539:GLU:C	2.58	0.47
1:B:130:GLY:O	1:B:446:ARG:NH1	2.47	0.47
1:B:229:LEU:C	1:B:231:ALA:H	2.22	0.47
1:B:505:THR:HG21	1:B:571:VAL:HG21	1.97	0.47
1:A:245:LEU:HB2	1:A:327:ALA:HB3	1.96	0.47
1:B:210:ILE:HD11	1:B:381:ILE:HD12	1.96	0.47
1:B:211:PHE:HB2	1:B:351:LEU:HD23	1.96	0.47
1:A:182:ALA:HA	1:A:202:LEU:O	2.15	0.47
1:A:538:LEU:HD12	1:A:539:GLU:OE2	2.15	0.47
1:A:15:ILE:CD1	1:A:505:THR:HB	2.45	0.47
1:A:82:SER:O	1:A:243:LYS:NZ	2.41	0.47
1:A:397:LEU:HD12	1:A:397:LEU:N	2.30	0.47
1:A:571:VAL:HG13	1:A:572:VAL:N	2.30	0.47
1:A:133:MET:HE2	1:A:133:MET:CA	2.44	0.46
1:B:132:PRO:O	1:B:363:LYS:CD	2.61	0.46
1:B:84:ALA:HB1	1:B:141:VAL:HG22	1.97	0.46
1:A:84:ALA:HB3	1:A:141:VAL:O	2.16	0.46
1:B:198:PHE:HE2	1:B:200:ARG:HG2	1.80	0.46
1:B:334:ASN:O	1:B:359:MET:HG2	2.15	0.46
1:A:504:LEU:N	1:A:504:LEU:HD22	2.30	0.46
1:B:81:LEU:HD22	1:B:331:ARG:HB2	1.96	0.46
1:B:87:ASP:HA	1:B:138:ASN:OD1	2.14	0.46
1:A:18:ARG:NH2	1:A:185:ASP:OD2	2.49	0.46
1:A:171:LEU:HB2	1:A:180:GLY:O	2.15	0.46
1:A:419:ARG:HG2	1:A:420:ASN:N	2.29	0.46
1:A:565:SER:O	1:A:566:GLN:C	2.58	0.46
1:B:73:ALA:CB	1:B:79:HIS:CE1	2.99	0.46
1:B:487:SER:O	1:B:490:ALA:HB3	2.16	0.46
1:A:386:THR:O	1:A:386:THR:CG2	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:PRO:O	1:B:99:LYS:HE3	2.15	0.46
1:B:495:ASN:C	1:B:495:ASN:ND2	2.74	0.46
1:B:360:ASN:HB3	1:B:365:LYS:O	2.16	0.46
1:B:494:THR:O	1:B:494:THR:HG23	2.16	0.46
1:B:516:ASN:HB3	1:B:524:GLU:OE2	2.15	0.46
1:B:31:ARG:NH1	1:B:200:ARG:NH2	2.63	0.46
1:B:218:HIS:ND1	1:B:219:LEU:N	2.64	0.46
1:A:24:TRP:CZ3	1:A:29:MET:HE1	2.51	0.46
1:B:135:ASN:HA	1:B:138:ASN:ND2	2.31	0.46
1:B:345:THR:HB	1:B:398:HIS:CD2	2.51	0.46
1:B:391:GLN:O	1:B:392:SER:OG	2.27	0.46
1:B:508:ASP:O	1:B:567:ASN:ND2	2.47	0.46
1:B:563:ASP:OD2	1:B:568:ILE:HG13	2.15	0.46
1:A:133:MET:CE	1:A:133:MET:CA	2.89	0.46
1:A:181:ILE:HD12	1:A:181:ILE:C	2.41	0.45
1:B:367:THR:OG1	3:B:613:FAD:H2'	2.15	0.45
1:A:288:LEU:CD2	1:A:320:LEU:HD21	2.46	0.45
1:B:44:GLY:O	1:B:45:PRO:C	2.59	0.45
1:B:53:ARG:HG2	1:B:378:ALA:HB3	1.98	0.45
1:A:419:ARG:HD2	1:A:452:THR:HG23	1.99	0.45
1:B:325:ARG:HD3	1:B:483:PHE:CE2	2.51	0.45
1:A:220:ALA:HA	1:A:223:LEU:HB2	1.99	0.45
1:B:181:ILE:HG23	1:B:182:ALA:N	2.30	0.45
1:A:114:PHE:HB2	1:A:127:ILE:HD11	1.98	0.45
1:A:296:TYR:CE2	1:A:562:LYS:HE2	2.52	0.45
1:A:539:GLU:CD	1:A:539:GLU:N	2.73	0.45
1:B:367:THR:O	1:B:371:MET:HG3	2.17	0.45
1:A:178:VAL:HG21	1:A:346:PHE:HE1	1.81	0.45
1:B:33:ALA:HB1	1:B:203:GLU:O	2.16	0.45
1:B:55:LYS:CG	1:B:159:VAL:HG12	2.32	0.45
1:B:72:LYS:HE2	1:B:555:HIS:HD2	1.78	0.45
1:B:244:GLU:CD	1:B:325:ARG:HD2	2.41	0.45
1:A:227:PHE:O	1:A:228:ASP:C	2.60	0.45
1:A:440:ILE:CG2	1:A:441:PHE:N	2.70	0.45
1:B:188:ILE:CG2	1:B:189:GLN:N	2.80	0.45
1:B:422:ARG:N	1:B:423:PRO:HD2	2.31	0.45
1:A:18:ARG:NH1	5:A:701:HOH:O	2.50	0.45
1:A:538:LEU:HD12	1:A:539:GLU:CD	2.42	0.45
1:A:555:HIS:N	1:A:555:HIS:CD2	2.83	0.45
1:B:165:TYR:CD2	1:B:184:ASN:OD1	2.70	0.45
1:B:227:PHE:O	1:B:228:ASP:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:LEU:CD2	1:B:532:VAL:HG11	2.47	0.45
1:A:9:ILE:HG13	1:A:9:ILE:H	1.44	0.45
1:A:503:HIS:HB2	1:A:571:VAL:O	2.17	0.45
1:A:294:LEU:CD1	1:A:558:THR:HG23	2.46	0.44
1:A:7:PRO:O	1:A:8:ARG:HB2	2.15	0.44
1:B:236:GLN:OE1	1:B:336:GLY:HA3	2.17	0.44
1:B:539:GLU:H	1:B:539:GLU:HG3	1.53	0.44
1:A:238:TYR:CG	1:A:561:ILE:HD13	2.51	0.44
1:A:514:ASN:O	1:A:518:SER:CB	2.65	0.44
1:B:364:ILE:O	1:B:364:ILE:CG1	2.65	0.44
1:B:506:LEU:HD23	1:B:512:PRO:HG2	2.00	0.44
1:A:21:ASP:OD1	1:A:24:TRP:HD1	2.01	0.44
1:A:364:ILE:O	1:A:364:ILE:HG22	2.17	0.44
1:B:293:GLY:C	1:B:295:ASP:H	2.24	0.44
1:B:541:GLY:O	1:B:542:ASP:C	2.59	0.44
1:B:117:LEU:HD22	1:B:313:HIS:CE1	2.53	0.44
1:B:278:HIS:CE1	1:B:286:LEU:HD11	2.52	0.44
1:A:135:ASN:HA	1:A:138:ASN:HD22	1.82	0.44
1:B:306:GLU:OE1	1:B:306:GLU:HA	2.17	0.44
1:B:72:LYS:HB3	1:B:72:LYS:HZ3	1.83	0.44
1:A:31:ARG:NE	1:A:200:ARG:NH1	2.66	0.44
1:A:86:LEU:HD22	1:A:87:ASP:N	2.33	0.44
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.79	0.44
1:B:21:ASP:HB3	1:B:24:TRP:CD1	2.50	0.44
1:B:242:LEU:CD2	1:B:304:PHE:HA	2.46	0.44
1:B:347:PRO:HA	1:B:398:HIS:HB2	2.00	0.44
1:A:86:LEU:N	1:A:139:TYR:O	2.39	0.44
1:A:189:GLN:HG3	1:A:191:ASP:OD2	2.18	0.44
1:B:245:LEU:HB2	1:B:327:ALA:HB3	2.00	0.44
1:B:392:SER:OG	1:B:393:LYS:N	2.51	0.44
1:A:325:ARG:HD3	1:A:491:LEU:CD1	2.46	0.43
1:B:132:PRO:C	1:B:134:ASN:H	2.25	0.43
1:B:307:PHE:O	1:B:307:PHE:CD1	2.70	0.43
1:B:335:GLU:HA	1:B:361:VAL:CG2	2.44	0.43
1:B:382:PHE:CE1	1:B:386:THR:HG21	2.53	0.43
1:B:154:ALA:O	1:B:159:VAL:HG22	2.17	0.43
1:B:167:ALA:CB	1:B:181:ILE:HG21	2.48	0.43
1:B:167:ALA:HB1	1:B:181:ILE:HG21	2.00	0.43
1:B:179:LYS:CE	1:B:205:HIS:NE2	2.81	0.43
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.80	0.43
1:B:406:LEU:C	1:B:408:ASN:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG12	1:A:163:PRO:HD3	2.00	0.43
1:B:392:SER:HB2	1:B:394:THR:OG1	2.18	0.43
1:B:498:HIS:HE1	1:B:551:GLN:HE21	1.64	0.43
1:B:536:VAL:HA	1:B:537:PRO:HD2	1.72	0.43
1:B:8:ARG:NH1	1:B:8:ARG:CG	2.76	0.43
1:B:529:PRO:HD2	2:B:612:SF4:S3	2.58	0.43
1:B:554:VAL:HG22	2:B:612:SF4:S1	2.58	0.43
1:A:48:LEU:CD1	1:A:147:VAL:HG13	2.49	0.43
1:B:165:TYR:HD2	1:B:184:ASN:OD1	2.02	0.43
1:B:198:PHE:CD2	1:B:198:PHE:C	2.96	0.43
1:B:442:TYR:HA	1:B:447:GLY:H	1.82	0.43
1:B:143:LEU:O	1:B:147:VAL:HG23	2.19	0.43
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.89	0.43
1:B:171:LEU:CB	1:B:179:LYS:HB3	2.49	0.43
1:A:21:ASP:OD1	1:A:24:TRP:CD1	2.72	0.43
1:A:399:VAL:HG12	1:A:399:VAL:O	2.19	0.43
1:B:148:SER:O	1:B:149:TRP:C	2.60	0.43
1:B:331:ARG:HD2	1:B:332:ALA:H	1.83	0.43
1:B:52:THR:HG21	1:B:95:PHE:CE1	2.54	0.42
1:B:109:VAL:HG13	1:B:258:VAL:HG13	2.01	0.42
1:B:276:LEU:HD21	1:B:286:LEU:HG	2.00	0.42
1:B:355:SER:N	1:B:356:PRO:CD	2.82	0.42
1:A:62:GLU:O	1:A:62:GLU:HG3	2.18	0.42
1:B:173:HIS:HB3	1:B:175:ASP:OD1	2.19	0.42
1:B:154:ALA:C	1:B:159:VAL:HG22	2.44	0.42
1:B:173:HIS:CB	1:B:175:ASP:OD1	2.68	0.42
1:B:496:HIS:CD2	1:B:578:GLY:N	2.81	0.42
1:A:5:LYS:HD3	1:A:6:VAL:H	1.85	0.42
1:A:244:GLU:HG2	1:A:307:PHE:HZ	1.85	0.42
1:A:288:LEU:HD21	1:A:320:LEU:HD21	2.01	0.42
1:B:132:PRO:O	1:B:134:ASN:N	2.48	0.42
1:B:195:LYS:HB3	1:B:198:PHE:N	2.34	0.42
1:B:496:HIS:HD2	1:B:577:GLY:CA	2.28	0.42
1:B:130:GLY:CA	1:B:446:ARG:HH12	2.33	0.42
1:B:154:ALA:C	1:B:156:ALA:N	2.77	0.42
1:B:362:PRO:HG3	1:B:421:ILE:HD12	2.01	0.42
1:B:569:ASN:O	1:B:571:VAL:HG23	2.19	0.42
1:B:244:GLU:HG2	1:B:307:PHE:CZ	2.55	0.42
1:B:301:LEU:HD23	1:B:301:LEU:C	2.43	0.42
1:B:128:LEU:O	1:B:130:GLY:N	2.53	0.42
1:B:279:LEU:HD13	1:B:279:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ARG:HA	1:A:305:ARG:HD2	1.81	0.42
1:A:544:PHE:CD1	1:A:544:PHE:N	2.88	0.42
1:B:130:GLY:C	1:B:446:ARG:HH12	2.28	0.42
1:B:362:PRO:HG3	1:B:418:VAL:HB	2.02	0.41
1:B:541:GLY:C	1:B:543:GLY:N	2.78	0.41
1:B:218:HIS:NE2	1:B:572:VAL:HG22	2.36	0.41
1:B:504:LEU:HD23	1:B:533:TYR:CZ	2.55	0.41
1:B:244:GLU:CB	1:B:327:ALA:O	2.68	0.41
1:B:537:PRO:HA	1:B:544:PHE:CD2	2.55	0.41
1:A:18:ARG:H	1:A:18:ARG:HG2	1.60	0.41
1:A:536:VAL:HG11	1:A:545:ARG:NH1	2.36	0.41
1:B:30:GLU:H	1:B:200:ARG:HD3	1.85	0.41
1:A:81:LEU:HD13	1:A:581:TYR:CZ	2.55	0.41
1:A:365:LYS:HA	3:A:611:FAD:C2	2.51	0.41
1:B:213:GLU:HG2	3:B:613:FAD:N7A	2.35	0.41
1:B:216:HIS:CD2	1:B:561:ILE:CG1	3.03	0.41
1:B:325:ARG:HH21	1:B:488:SER:HA	1.72	0.41
1:B:393:LYS:O	1:B:394:THR:HG23	2.19	0.41
1:B:503:HIS:CD2	1:B:503:HIS:N	2.89	0.41
1:A:87:ASP:HA	1:A:88:PRO:HD3	1.83	0.41
1:A:310:TRP:NE1	1:A:316:ILE:HD13	2.36	0.41
1:B:95:PHE:CD2	1:B:149:TRP:CZ3	3.08	0.41
1:B:505:THR:CG2	1:B:571:VAL:HG23	2.51	0.41
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.73	0.41
1:A:546:LEU:HG	1:A:547:GLN:N	2.35	0.41
1:B:230:ARG:NH1	1:B:233:CYS:SG	2.93	0.41
1:A:246:TRP:CZ2	1:A:325:ARG:HB2	2.56	0.41
1:A:384:GLN:NE2	1:A:399:VAL:HG22	2.36	0.41
1:B:307:PHE:CD1	1:B:307:PHE:C	2.95	0.41
1:B:528:CYS:SG	1:B:532:VAL:HB	2.60	0.41
1:A:382:PHE:O	1:A:386:THR:HB	2.21	0.41
1:B:210:ILE:HD11	1:B:381:ILE:CD1	2.51	0.41
1:B:306:GLU:CD	1:B:474:TYR:HE2	2.28	0.41
1:B:325:ARG:HH21	1:B:491:LEU:HD12	1.86	0.41
1:A:48:LEU:HD12	1:A:147:VAL:HG13	2.03	0.41
1:A:244:GLU:HG2	1:A:307:PHE:CZ	2.55	0.41
1:B:149:TRP:CZ3	1:B:153:GLN:HG3	2.56	0.41
1:B:157:LEU:HD22	1:B:157:LEU:HA	1.89	0.41
1:A:359:MET:HE3	1:A:364:ILE:HA	2.02	0.40
1:A:573:PRO:O	1:A:574:GLU:C	2.62	0.40
1:B:10:THR:O	1:B:16:TYR:CE1	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:CD1	1:B:506:LEU:O	2.69	0.40
1:B:240:ILE:HD13	1:B:303:PRO:HB2	2.04	0.40
1:B:318:PRO:HA	1:B:321:GLU:HB2	2.03	0.40
1:B:522:GLY:O	1:B:525:GLN:HG3	2.21	0.40
1:A:69:LEU:CD1	1:A:69:LEU:C	2.93	0.40
1:A:189:GLN:O	1:A:190:LYS:C	2.64	0.40
1:B:132:PRO:HD3	1:B:442:TYR:CE2	2.57	0.40
1:A:253:TRP:O	1:A:254:LYS:HE3	2.21	0.40
1:B:31:ARG:NH1	1:B:182:ALA:HB1	2.37	0.40
1:B:186:VAL:CG1	1:B:187:GLY:N	2.82	0.40
1:B:264:TRP:CG	1:B:265:PRO:HA	2.57	0.40
1:B:536:VAL:O	1:B:544:PHE:CA	2.67	0.40
1:B:72:LYS:HD2	1:B:570:TRP:HH2	1.86	0.40
1:B:98:TRP:CZ3	1:B:105:LEU:HB2	2.56	0.40
1:B:229:LEU:CD2	1:B:343:LYS:HB3	2.51	0.40
1:A:69:LEU:C	1:A:69:LEU:HD13	2.47	0.40
1:A:115:GLY:O	1:A:261:THR:HA	2.21	0.40
1:A:202:LEU:CD1	1:A:203:GLU:N	2.85	0.40
1:B:18:ARG:HD2	1:B:18:ARG:H	1.86	0.40
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.97	0.40
1:B:416:TYR:O	1:B:419:ARG:HD3	2.21	0.40
1:B:557:LYS:HE2	1:B:570:TRP:CZ3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/584 (99%)	528 (91%)	38 (7%)	13 (2%)	5	10
1	B	576/584 (99%)	497 (86%)	58 (10%)	21 (4%)	2	4
All	All	1155/1168 (99%)	1025 (89%)	96 (8%)	34 (3%)	3	6

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	GLU
1	B	8	ARG
1	B	20	GLN
1	B	74	ALA
1	B	129	PRO
1	B	194	PRO
1	B	393	LYS
1	B	395	ILE
1	B	538	LEU
1	B	544	PHE
1	A	389	ASN
1	A	394	THR
1	B	99	LYS
1	B	133	MET
1	B	394	THR
1	B	532	VAL
1	A	62	GLU
1	A	294	LEU
1	A	387	SER
1	A	539	GLU
1	B	392	SER
1	B	539	GLU
1	B	30	GLU
1	B	164	GLY
1	B	537	PRO
1	A	440	ILE
1	B	88	PRO
1	A	347	PRO
1	A	356	PRO
1	A	6	VAL
1	A	364	ILE
1	B	573	PRO
1	B	364	ILE
1	A	7	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	482/486 (99%)	424 (88%)	58 (12%)	5	10
1	B	479/486 (99%)	398 (83%)	81 (17%)	2	4
All	All	961/972 (99%)	822 (86%)	139 (14%)	3	6

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	5	LYS
1	A	6	VAL
1	A	8	ARG
1	A	9	ILE
1	A	18	ARG
1	A	19	ASP
1	A	21	ASP
1	A	22	LYS
1	A	23	ARG
1	A	29	MET
1	A	35	GLU
1	A	53	ARG
1	A	57	LEU
1	A	69	LEU
1	A	72	LYS
1	A	81	LEU
1	A	86	LEU
1	A	89	ARG
1	A	97	ASP
1	A	99	LYS
1	A	107	THR
1	A	122	ARG
1	A	133	MET
1	A	134	ASN
1	A	140	VAL
1	A	174	GLU
1	A	190	LYS
1	A	200	ARG
1	A	202	LEU
1	A	219	LEU
1	A	223	LEU
1	A	225	LYS
1	A	237	THR

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Mol	Chain	Res	Type
1	A	240	ILE
1	A	252	LYS
1	A	254	LYS
1	A	266	LEU
1	A	279	LEU
1	A	286	LEU
1	A	320	LEU
1	A	321	GLU
1	A	325	ARG
1	A	363	LYS
1	A	386	THR
1	A	387	SER
1	A	401	GLU
1	A	419	ARG
1	A	422	ARG
1	A	449	GLU
1	A	462	GLN
1	A	467	LYS
1	A	511	VAL
1	A	515	ARG
1	A	526	ARG
1	A	542	ASP
1	A	551	GLN
1	A	571	VAL
1	B	18	ARG
1	B	20	GLN
1	B	23	ARG
1	B	25	GLU
1	B	30	GLU
1	B	31	ARG
1	B	37	ASP
1	B	53	ARG
1	B	60	GLN
1	B	64	ASP
1	B	67	VAL
1	B	69	LEU
1	B	70	VAL
1	B	71	GLU
1	B	72	LYS
1	B	86	LEU
1	B	94	LEU
1	B	99	LYS

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Mol	Chain	Res	Type
1	B	101	LYS
1	B	133	MET
1	B	141	VAL
1	B	152	GLU
1	B	157	LEU
1	B	159	VAL
1	B	161	VAL
1	B	165	TYR
1	B	174	GLU
1	B	178	VAL
1	B	189	GLN
1	B	191	ASP
1	B	195	LYS
1	B	197	THR
1	B	199	GLU
1	B	202	LEU
1	B	209	THR
1	B	218	HIS
1	B	222	GLN
1	B	240	ILE
1	B	250	GLU
1	B	252	LYS
1	B	258	VAL
1	B	259	ASP
1	B	266	LEU
1	B	279	LEU
1	B	283	GLU
1	B	286	LEU
1	B	331	ARG
1	B	333	LEU
1	B	344	LEU
1	B	350	LEU
1	B	363	LYS
1	B	376	LEU
1	B	380	SER
1	B	383	ASN
1	B	390	LEU
1	B	393	LYS
1	B	394	THR
1	B	395	ILE
1	B	401	GLU
1	B	403	GLU

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Mol	Chain	Res	Type
1	B	422	ARG
1	B	448	MET
1	B	449	GLU
1	B	452	THR
1	B	461	ASP
1	B	462	GLN
1	B	467	LYS
1	B	485	LEU
1	B	495	ASN
1	B	503	HIS
1	B	505	THR
1	B	511	VAL
1	B	513	VAL
1	B	524	GLU
1	B	527	PHE
1	B	538	LEU
1	B	539	GLU
1	B	542	ASP
1	B	544	PHE
1	B	551	GLN
1	B	574	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	60	GLN
1	A	61	HIS
1	A	145	HIS
1	A	153	GLN
1	A	173	HIS
1	A	184	ASN
1	A	189	GLN
1	A	280	ASN
1	A	384	GLN
1	A	389	ASN
1	A	516	ASN
1	A	525	GLN
1	A	540	GLN
1	A	551	GLN
1	A	552	ASN
1	B	60	GLN

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Mol	Chain	Res	Type
1	B	61	HIS
1	B	138	ASN
1	B	278	HIS
1	B	334	ASN
1	B	368	HIS
1	B	462	GLN
1	B	495	ASN
1	B	498	HIS
1	B	516	ASN
1	B	525	GLN
1	B	552	ASN
1	B	555	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	A	610	1	0,12,12	-	-	-		
4	TBU	A	621	-	4,4,4	0.45	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	611	-	58,58,58	2.31	18 (31%)	85,89,89	1.55	12 (14%)
4	TBU	A	622	-	4,4,4	0.36	0	6,6,6	0.60	0
4	TBU	B	625	-	4,4,4	0.53	0	6,6,6	0.45	0
2	SF4	B	612	1	0,12,12	-	-	-	-	-
4	TBU	A	624	-	4,4,4	0.40	0	6,6,6	0.58	0
3	FAD	B	613	-	58,58,58	2.18	15 (25%)	85,89,89	1.67	15 (17%)
4	TBU	B	626	-	4,4,4	0.54	0	6,6,6	0.48	0
4	TBU	A	623	-	4,4,4	0.70	0	6,6,6	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	613	-	-	7/34/50/50	0/6/6/6
3	FAD	A	611	-	-	2/34/50/50	0/6/6/6
2	SF4	A	610	1	-	-	0/6/5/5
2	SF4	B	612	1	-	-	0/6/5/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	FAD	PA-O3P	-8.89	1.49	1.59
3	B	613	FAD	PA-O3P	-7.63	1.51	1.59
3	B	613	FAD	C10-N10	5.81	1.49	1.37
3	A	611	FAD	C1'-C2'	-5.69	1.44	1.52
3	B	613	FAD	C6-C5X	4.85	1.47	1.40
3	A	611	FAD	C10-N10	4.66	1.47	1.37
3	B	613	FAD	C9A-N10	4.48	1.48	1.41
3	A	611	FAD	C9A-N10	4.21	1.48	1.41
3	A	611	FAD	C4X-N5	4.07	1.39	1.30
3	B	613	FAD	C4X-N5	3.95	1.39	1.30
3	B	613	FAD	C4A-N3A	3.87	1.41	1.34
3	A	611	FAD	O4B-C4B	-3.86	1.36	1.45
3	A	611	FAD	C9-C9A	3.46	1.45	1.39
3	B	613	FAD	C9-C9A	3.41	1.45	1.39
3	B	613	FAD	C10-N1	3.39	1.40	1.33
3	A	611	FAD	C1'-N10	-3.39	1.39	1.47
3	B	613	FAD	C1'-C2'	-3.34	1.48	1.52
3	B	613	FAD	P-O3P	3.24	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	FAD	C6-C5X	3.20	1.44	1.40
3	A	611	FAD	C9A-C5X	2.95	1.45	1.41
3	A	611	FAD	P-O5'	-2.91	1.48	1.59
3	B	613	FAD	C9A-C5X	2.83	1.45	1.41
3	B	613	FAD	O4B-C4B	-2.62	1.39	1.45
3	A	611	FAD	C4-N3	2.46	1.43	1.38
3	A	611	FAD	C8A-N9A	2.42	1.41	1.37
3	B	613	FAD	C8-C7	2.37	1.46	1.40
3	A	611	FAD	C8-C7	2.31	1.46	1.40
3	B	613	FAD	C4'-C3'	2.30	1.57	1.53
3	B	613	FAD	C4-N3	2.20	1.43	1.38
3	A	611	FAD	C9-C8	-2.16	1.36	1.39
3	A	611	FAD	C4A-N9A	-2.15	1.33	1.37
3	A	611	FAD	O3B-C3B	2.15	1.48	1.43
3	A	611	FAD	C4A-N3A	2.10	1.38	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	613	FAD	O3'-C3'-C2'	8.22	127.61	108.93
3	A	611	FAD	O3'-C3'-C2'	6.52	123.74	108.93
3	B	613	FAD	P-O5'-C5'	4.61	147.77	121.35
3	A	611	FAD	P-O5'-C5'	4.57	147.53	121.35
3	B	613	FAD	O4B-C1B-C2B	-3.64	98.83	106.62
3	A	611	FAD	O2-C2-N3	3.55	125.40	118.58
3	B	613	FAD	C9A-C5X-N5	3.55	126.22	122.45
3	A	611	FAD	C9A-C5X-N5	3.48	126.15	122.45
3	B	613	FAD	O4'-C4'-C3'	3.38	117.16	109.25
3	A	611	FAD	O4B-C1B-C2B	-3.21	99.74	106.62
3	B	613	FAD	C2'-C1'-N10	3.12	124.92	110.20
3	A	611	FAD	O2-C2-N1	-2.95	116.90	121.80
3	A	611	FAD	C2'-C1'-N10	2.94	124.10	110.20
3	A	611	FAD	O4'-C4'-C3'	2.76	115.71	109.25
3	A	611	FAD	C5X-C9A-N10	-2.66	115.56	117.97
3	B	613	FAD	C5X-C9A-N10	-2.64	115.58	117.97
3	B	613	FAD	O2-C2-N3	2.64	123.64	118.58
3	B	613	FAD	C5'-C4'-C3'	-2.63	107.25	112.22
3	B	613	FAD	C3B-C2B-C1B	2.59	106.37	101.46
3	B	613	FAD	C9-C9A-N10	2.53	125.26	121.85
3	A	611	FAD	O3'-C3'-C4'	-2.48	103.30	108.93
3	A	611	FAD	C9-C9A-N10	2.39	125.07	121.85
3	B	613	FAD	O3'-C3'-C4'	-2.33	103.64	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	611	FAD	C3B-C2B-C1B	2.29	105.80	101.46
3	B	613	FAD	C4B-O4B-C1B	2.29	114.52	109.47
3	B	613	FAD	C4-C4X-N5	-2.25	115.10	118.21
3	B	613	FAD	O5'-C5'-C4'	2.02	114.76	109.36

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	611	FAD	PA-O3P-P-O5'
3	B	613	FAD	O2'-C2'-C3'-O3'
3	B	613	FAD	C2'-C3'-C4'-O4'
3	B	613	FAD	PA-O3P-P-O5'
3	B	613	FAD	C2'-C3'-C4'-C5'
3	B	613	FAD	C1'-C2'-C3'-O3'
3	A	611	FAD	O4B-C4B-C5B-O5B
3	B	613	FAD	PA-O3P-P-O2P
3	B	613	FAD	O4B-C4B-C5B-O5B

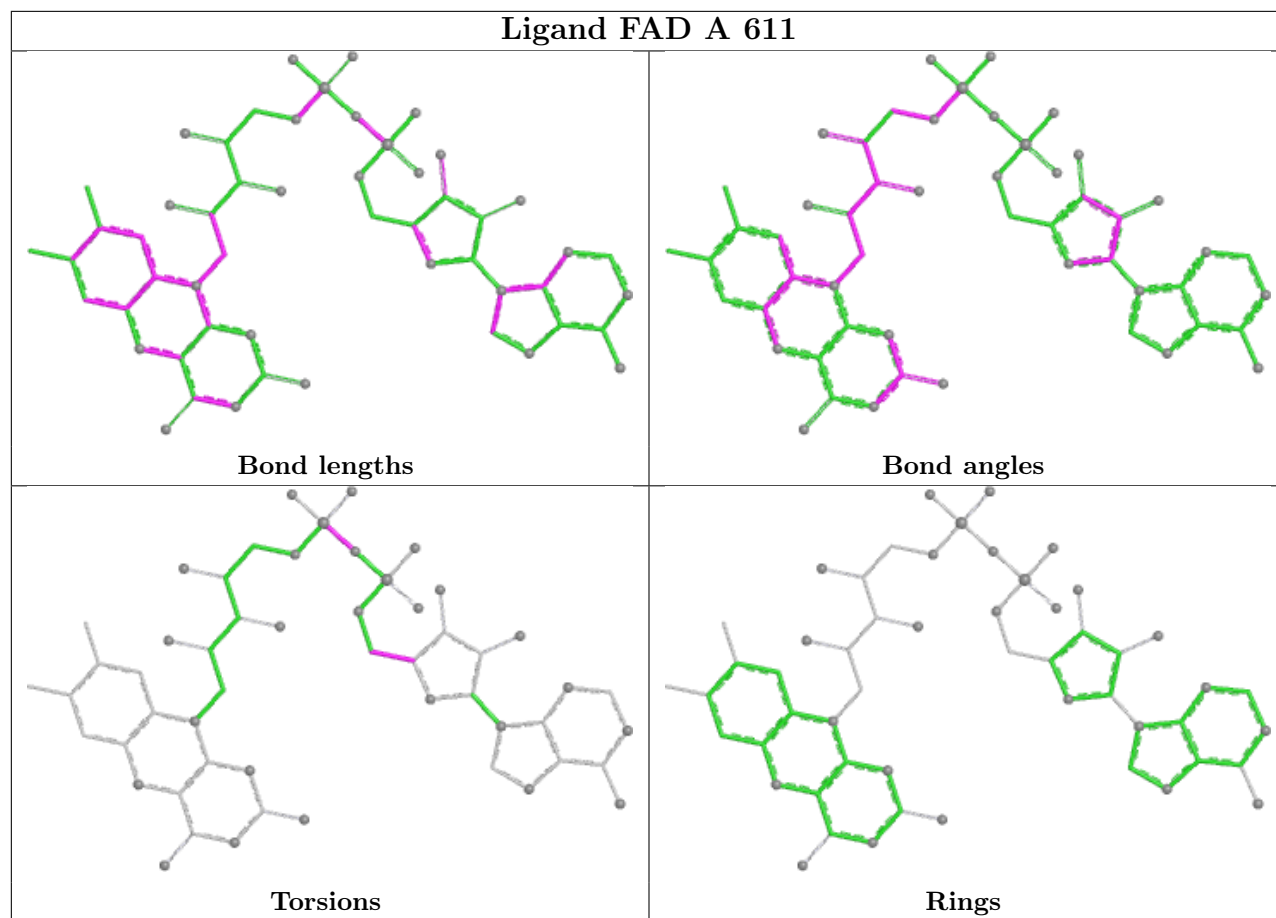
There are no ring outliers.

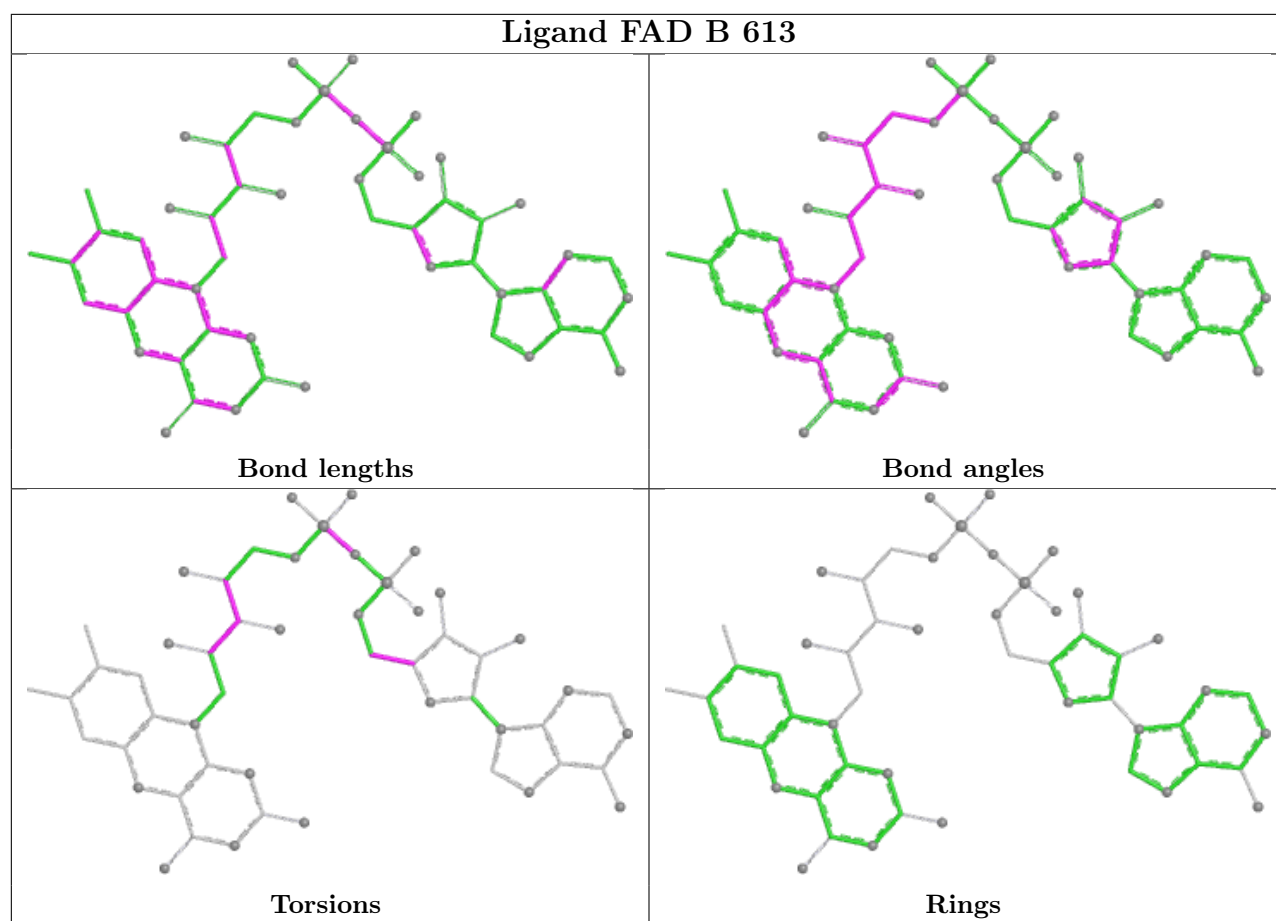
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	621	TBU	3	0
3	A	611	FAD	2	0
2	B	612	SF4	3	0
3	B	613	FAD	3	0
4	A	623	TBU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD A 611





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/584 (99%)	-0.51	6 (1%) 79 76	7, 23, 56, 89	0
1	B	578/584 (98%)	0.53	22 (3%) 44 38	29, 63, 85, 95	0
All	All	1159/1168 (99%)	0.01	28 (2%) 59 54	7, 45, 83, 95	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	PRO	5.7
1	A	6	VAL	5.0
1	B	131	LEU	4.3
1	B	132	PRO	3.9
1	A	131	LEU	3.7
1	B	165	TYR	3.3
1	B	27	VAL	3.1
1	B	133	MET	3.1
1	B	395	ILE	3.0
1	B	32	PHE	3.0
1	A	132	PRO	2.9
1	B	130	GLY	2.8
1	A	390	LEU	2.8
1	B	555	HIS	2.8
1	B	502	ALA	2.6
1	B	75	HIS	2.5
1	B	396	GLY	2.5
1	B	72	LYS	2.4
1	B	327	ALA	2.4
1	B	147	VAL	2.4
1	A	133	MET	2.3
1	B	80	THR	2.2
1	B	554	VAL	2.2
1	B	397	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	2.1
1	B	212	ALA	2.1
1	B	24	TRP	2.0
1	B	542	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

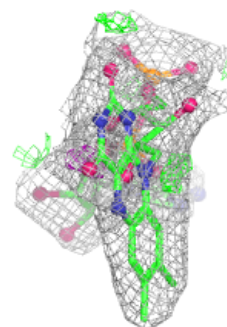
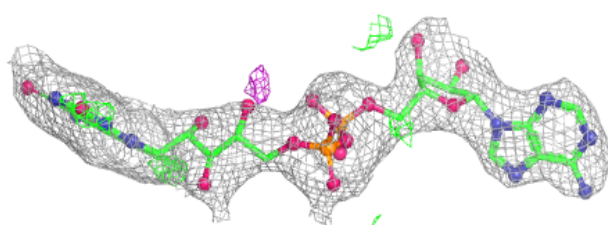
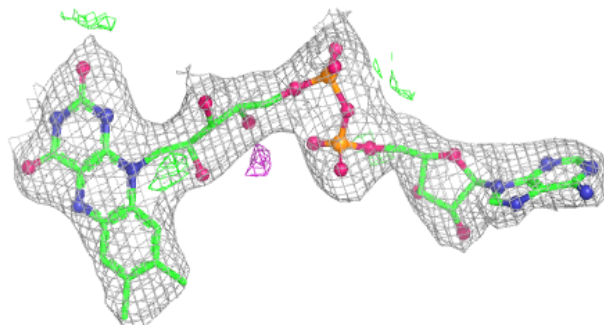
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TBU	B	626	5/5	0.76	0.29	57,57,59,59	0
4	TBU	A	623	5/5	0.83	0.21	29,33,34,38	0
3	FAD	B	613	53/53	0.90	0.10	42,58,74,74	0
4	TBU	A	622	5/5	0.91	0.12	26,27,28,28	0
4	TBU	A	624	5/5	0.92	0.17	51,51,51,52	0
4	TBU	B	625	5/5	0.93	0.16	56,56,57,57	0
4	TBU	A	621	5/5	0.93	0.11	25,25,27,28	0
2	SF4	B	612	8/8	0.96	0.07	51,53,54,54	0
3	FAD	A	611	53/53	0.98	0.05	7,13,20,21	0
2	SF4	A	610	8/8	0.98	0.05	6,8,9,10	0

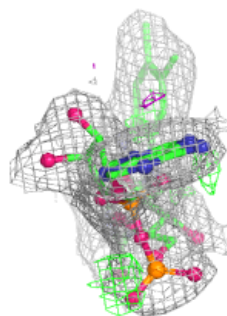
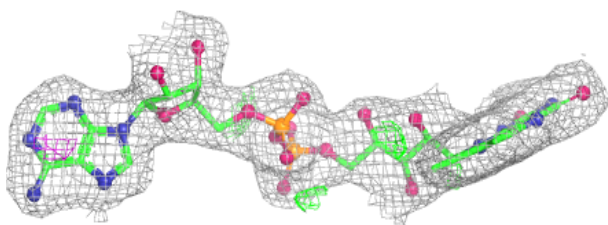
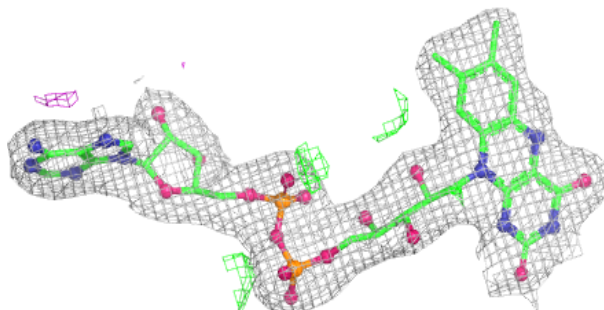
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD B 613:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 611:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.